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LARGE EDDY SIMULATIONS OF SUPERCRITICAL MIXING LAYERS BASED ON SUBGRID SCALE MODELS EXTRACTED FROM DIRECT NUMERICAL SIMULATIONS

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SUMMARY/OVERVIEW:

The objective of this study is the fundamental understanding of fuel disintegration and mixing in a supercritical environment (relative to the fuel) in order to determine parameter regimes advantageous to mixing. The approach is based on the future goal of developing a model for a supercritical, turbulent jet mixing with surrounding fluid. The method is one that combines the modeling of supercritical fluids with a systematic development based on the Large Eddy Simulation (LES) approach. This systematic development includes a consistent protocol based upon Direct Numerical Simulations (DNS) for developing a Subgrid Scale (SGS) Model appropriate to supercritical fluids, rather than choosing in an ad hoc manner an existing SGS model developed under assumptions inconsistent with supercritical fluid behavior. This SGS model should be used in future studies of supercritical turbulent jets utilizing the LES methodology.

TECHNICAL DISCUSSION

During this initial year, our activities focused on first deriving the correct Large Eddy Simulation (LES) conservation equations, through filtering, from the Direct Numerical Simulation (DNS) equations. These LES equations contain several types of terms; (1) terms which are akin to those of the DNS equations except that they are now functions of the filtered dependent variables, and thus are called "resolved" because the equations are solved at the scale of the filtered variables variation, (2) subgrid scale fluxes of momentum, enthalpy and species, and (3) terms that are gradients of the difference between a LES (i.e. filtered) quantity and the DNS mathematical form of the same quantity calculated as a function of the filtered variables, with other terms such as the difference between triple correlation terms also appearing in the energy equation. Type (1) terms are the basic terms in the LES equations. Type (2) terms are the classical subgrid scale (SGS) fluxes that are usually modeled in the LES equations to reproduce the behavior of the scales that have been filtered; below we discuss the modeling of these terms. Type (3) terms are usually neglected without justification other than to state that they are believed negligible – these are called "the LES assumptions"; we have found that for supercritical situations neglecting these terms is certainly not correct, as discussed below.

To evaluate the LES assumptions as well as to assess the mathematical form of the SGS fluxes, we used a DNS database of a temporal mixing layer portrayed in Fig. 1. The initial conditions for

the several DNS of the database are listed in Table 1, where p_r is the reduced pressure, which in all cases in approximately 2. In each DNS, a transitional state has been reached, and it is this transitional case that has been analyzed for SGS model development. The details of the DNS and the flow behavior have been described in detail in [1–3].

(i)LES assumptions. To analyze the terms in the LES equations, budgets of the filtered equations were calculated over the entire domain volume at the transitional states. It turns out that in the momentum equation, the leading terms are: the resolved convective term, the pressure gradient and the gradient of the difference between the LES pressure and the pressure computed using the real-gas equation of state (EOS) and the filtered variables. The next terms in order of magnitude are the resolved stresses, the subgrid stresses, and the gradient of the difference between the filtered stresses and the stresses calculated as a function of the filtered variables; these terms are at least an order of magnitude smaller than the leading terms. In the species equations, in decreasing order the leading terms are: convection, SGS flux and resolved flux which is of same order of magnitude as the gradient of the difference between the filtered flux of species and the flux calculated using the filtered variables. Similarly, in the energy equation, the convection term is the largest, followed by a group of terms at least an order of magnitude smaller: the pressure work, the SGS flux term and the gradient of the difference between the filtered heat flux and the heat flux computed as a function of the filtered variables. The next batch of terms in decreasing order of magnitude are the resolved viscous term, the gradient of the difference between the LES pressure and the pressure computed using the real-gas EOS and the filtered variables, and the triple correlation. The smallest terms are those resulting from the LES assumptions on the triple correlations and the stresses. It is thus clear that terms so far neglected in **ALL** existing LES under supercritical conditions are important in that they are of same magnitude as resolved terms. Because the budget represents a volumetric average, it is also clear that locally, at the high density-gradient-magnitude regions identified in all supercritical turbulent flows, both in DNS [1–3] and in experiments (e.g. [4,5]), the contribution of the so far neglected terms in LES may be entirely dominating all other terms.

These conclusions indicated that modeling of novel terms must be undertaken. As a model, expressions for these terms are first sought for the pressure. The idea was thus to employ a Taylor expansion of the pressure around the filtered set of variables as a representation of the large gradient differences between filtered and EOS pressure computed using the filtered quantity. However, the EOS is function of (v, X, T), v the molar volume, X the molar fraction and T the temperature, whereas the conservation equations are solved for the conservative variables. Moreover, the thermodynamic related variances that are modeled in the SGS fluxes are associated with the mass fraction Y and the enthalpy H rather than the intrinsic thermodynamic variables (v, X, T). The quandary as to the choice of the appropriate variables for the Taylor expansion, with several possibilities tried, occupied a considerable portion of time, as did the derivation of the Jacobian for the change of variables from one set of dependent variables to another. Handling of the very large DNS datasets with the uncertain set of variables for the Taylor expansion also proved very difficult. It was finally decided to adopt a one-dimensional problem as a test case for assessing the Taylor expansion effectiveness for several sets of variables. In this problem, the X and T profiles are prescribed through a hyperbolic tangent as a function of an index in such a manner that p calculated through the EOS is constant. Results of the assessment are shown in Fig. 2. In Fig. 2a one can see that the Taylor series expansion in the variables (v, X, T) is a much better approximation of the filtered p than is p computed from the EOS as a function of the filtered variables, and this holds whether the Taylor expansion is calculated analytically or numerically; therefore the principle of the Taylor

expansion for such calculation is validated. Figure 2b shows that the set $(\rho,\ Y,\ H)$ is not as appropriate as the set $(\rho,\ \rho Y,\ \rho E)$ for approximating the filtered pressure through the Taylor expansion. This observation indicates the set of variables to choose for the transformation from the intrinsic set, a task that is currently underway as a precursor for *a priori* assessment of the models on the databases.

An evaluation on the DNS database of a model previously used for the filtered triple correlation difference under atmospheric conditions [6] proved that the previous model remains valid under supercritical conditions.

(ii) **SGS fluxes.** Three models were tested for the SGS fluxes: (1) the Smagorinsky (SM) model with the trace computed using the Yoshizawa (YO) model, (2) the Scale Similarity (SS) model, and (3) the Gradient (GR) model of [7]. These tests were *a priori*, meaning that the mathematical form was tested (the correlation) and a proportionality coefficient was computed (through a least square fit) using the DNS database. An example of this assessment is shown in Fig. 3 for the SGS species flux for the OHe600 layer, which is that having the highest Reynolds number at transition. The assessment is shown for the larger of the two grid filters considered, and for the SS model at two test filters, model SS1 (test filter has same size as the grid filter) and SS2 (test filter is twice the size of the grid filter). The results are typical of the findings for all SGS fluxes. The SM model shows poor correlation with the exact SGS fluxes, while the GR and SS models have high correlations. Furthermore, the calibrated coefficients for the GR and SS models yielded good quantitative agreement with the SGS fluxes. However, comparison among the layers in the DNS database revealed that statistically, the calibrated coefficients were not generally valid, indicating that most likely a dynamic strategy would be necessary for computing these coefficients in *a posteriori* calculations.

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Name	HN400	HN500	HN600	HN800	OH750	OH550	OH500	OHe600
Species 2	C_7H_{16}	C_7H_{16}	C_7H_{16}	C_7H_{16}	O_2	O_2	O_2	O_2
Species 1	N_2	N_2	N_2	N_2	H_2	H_2	H_2	He
T_2 (K)	600	600	600	600	400	400	235	235
T_1 (K)	1000	1000	1000	1000	600	600	287	287
ρ_1/ρ_2	12.88	12.88	12.88	12.88	24.4	24.4	24.51	12.17
p_0 (atm)	60	60	60	60	100	100	100	100
Re_0	400	500	600	800	750	550	500	600

Table 1. Initial conditions of the Direct Numerical Simulations (DNS) database. In all simulations $M_{c,0} = 0.4$, $\delta_{\omega,0} = 6.859 \times 10^{-3}$ m (see Fig. 1). For the C_7H_{16}/N_2 layers, $p_r = 2.22$ and $((\rho_2 U_2)/(\rho_1 U_1)) = 5.276$; for the O_2/H_2 layers, $p_r = 2.01$ and $((\rho_2 U_2)/(\rho_1 U_1)) = 5.001$ for OH550 and OH750, and $((\rho_2 U_2)/(\rho_1 U_1)) = 4.951$ for OH500 and for the O_2/He layer $p_r = 2.01$ and $((\rho_2 U_2)/(\rho_1 U_1)) = 3.500$.
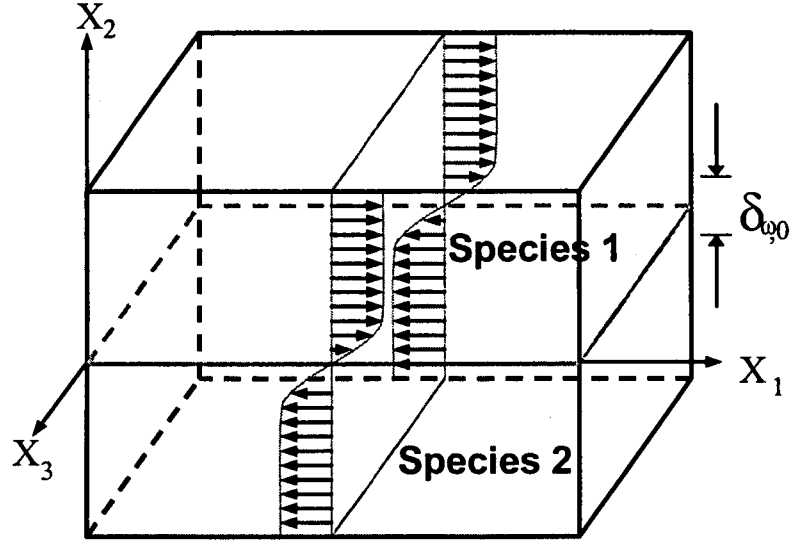
Figure 1. Mixing layer configuration for the DNS listed in Table 1.
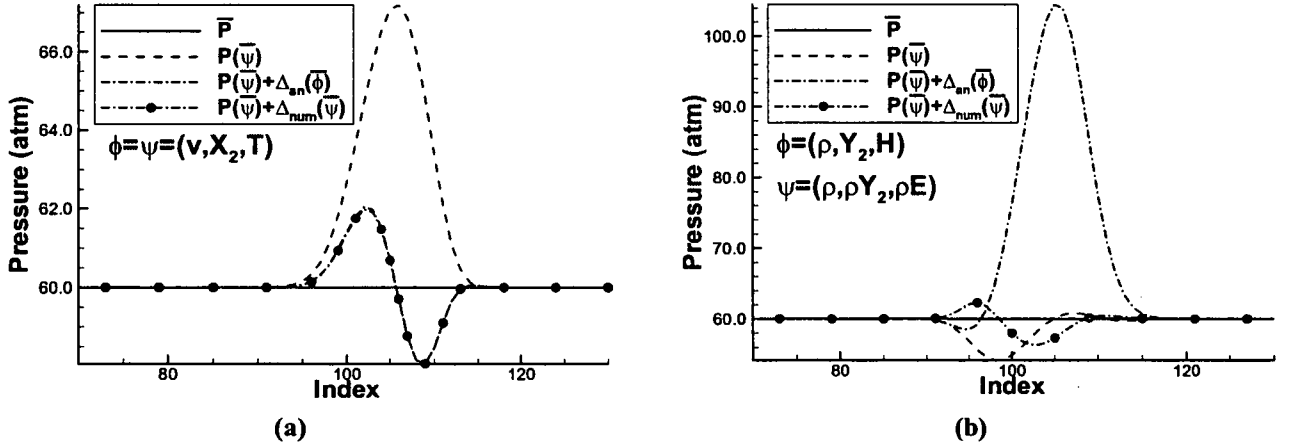

(a)   (b)

Figure 2. Filtered pressure and pressure computed as a function of the filtered field and pressure computed as a Taylor expansion of different sets of variables. (a) Intrinsic thermodynamic variables, (b) Two other sets of thermodynamic variables.
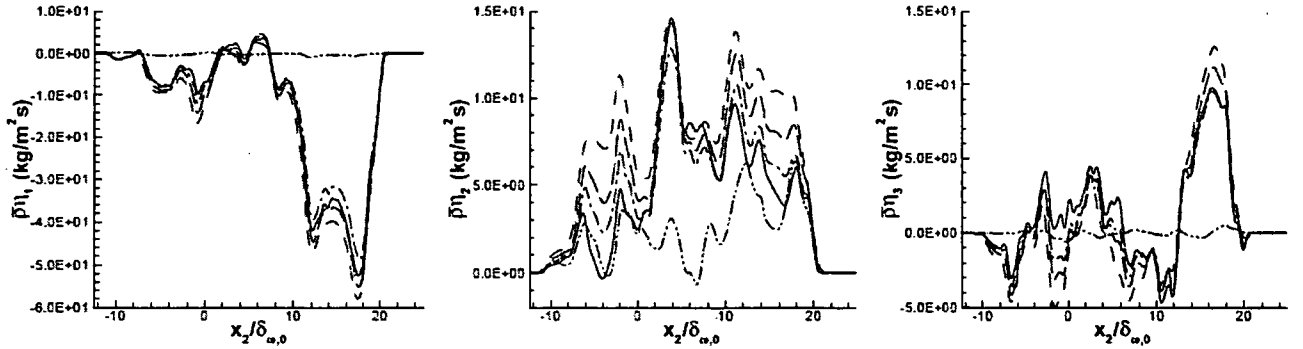

Figure 3. *A priori* assessment for the species SGS flux computed on the DNS database OHe600 (Table 1). The legend is: —— Exact; — τ — τ — GR, C_{GR}=0.1180; — τ τ — τ τ — SM, C_{SM}=0.0622; —— - — —— SS1, C_{SS1}=1.4671; — — — SS2, C_{SS2}=0.5369.